4-Phenylurazole

Other names:	1,2,4-Triazolidine-3,5-dione, 4-phenyl-
	4-Phenylurazol
	Bicarbamimide, N-phenyl-
	Urazole, 4-phenyl-
	4-phenyl-1,2,4-triazolidine-3,5-dione
Inchi:	InChI=1S/C8H7N3O2/c12-7-9-10-8(13)11(7)6-4-2-1-3-5-6/h1-5H,(H,9,12)(H,10,13)
InchiKey:	GOSUFRDROXZXLN-UHFFFAOYSA-N
Formula:	C8H7N3O2
SMILES:	O=c1[nH][nH]c(=O)n1-c1ccccc1
Mol. weight [g/mol]:	177.16
CAS:	15988-11-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.41		Crippen Method
logp	-1.110		Crippen Method
mcvol	122.040	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15988111&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume